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LASER SPECTROSCOPIC STUDIES OF MOLECULAR CRYSTALS.(U)
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1 June 1975 - 30 November 1979

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March 1980

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Electronic Raman scattering; magnetic phase transition; molecular solids; quadratic vibronic coupling; photochemistry; fluorescence; excited states; cryogenic liquid; energy transfer; phase transition; polariton; vibrational mixing (normal mode breakdown); degenerate electronic states.		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This report summarizes the work performed under the contract from 1 June 1975 to 30 November 1979. It includes a summary of new results, a list of all technical reports generated during the life of the contract, and a listing of personnel associated with the project.		

I. PERSONNEL WHO PARTICIPATED IN THE RESEARCH

1. Elliot R. Bernstein, Principal Investigator.
2. Daniel L. Michalopoulos, Graduate Student - Electronic Raman scattering and inorganic molecular vibronic coupling.
3. Gerald R. Meredith, Graduate Student - ReF_6 magnetic properties, vibronic coupling, electronic Raman scattering and crystal vibrational levels.
4. John D. Webb, Graduate Student - IrF_6 magnetic properties, vibronic coupling, electronic Raman scattering and crystal vibrational levels.
5. John D. Webb, Postdoctoral Fellow - Nonlinear optical phenomena, multiphoton spectroscopy and photochemistry of $\text{C}_3\text{N}_3\text{H}_3$.
6. Kerry M. Swift, Graduate Student - Nonlinear optical phenomena - multiphoton photochemistry and spectroscopy of OsO_4 , $\text{C}_3\text{N}_3\text{H}_3$.
7. Philip M. Kennedy, Graduate Student - Nonlinear optical phenomena - multiphoton photochemistry and spectroscopy of transition metal hexafluorides.
8. K. M. Chen, Graduate Student - Spectroscopy of rare earth borohydrides, vibronic transitions in rare earth compounds.

II. TECHNICAL REPORTS GENERATED

7. "Spectroscopic Properties of Rare Earth Borohydrides: $\text{Er}(\text{BH}_4)_3 \cdot 3\text{THF}$ in Pure and Mixed Crystals," E. R. Bernstein and K. M. Chen.
8. "Interactions in Inorganic Molecular Crystals - Electronic Spectra of ReF_6 Pure and Mixed Crystals," E. R. Bernstein and G. R. Meredith.
9. "Laser Optical Studies of Molecular Solids," E. R. Bernstein.
10. "On the Jahn Teller Effect in ReF_6 ," G. R. Meredith, J. D. Webb, and E. R. Bernstein.
11. "Raman Spectra of SiF_4 and GeF_4 Crystals," E. R. Bernstein and G. R. Meredith.
12. "Vibrational Spectra of Transition Metal Hexafluoride Crystals. I. Orthorhombic MoF_6 , WF_6 , and UF_6 Neat Crystals," E. R. Bernstein and G. R. Meredith.
13. "Vibrational Spectra of Transition Metal Hexafluoride Crystals. II. Two-Particle and Mixed Crystal Spectra as Techniques for Determination of Densities of States," E. R. Bernstein and G. R. Meredith.
14. "Vibrational Spectra of Transition Metal Hexafluoride Crystals. III. Exciton Band Structures of MoF_6 , WF_6 and UF_6 ," E. R. Bernstein and G. R. Meredith.

II. (Continued)

15. "On the Jahn Teller Effect in IrF_6 : The $\Gamma_{8g} (t_{2g})^3$ State at 6800 \AA ," E. R. Bernstein and J. D. Webb.
16. "Charge-Transfer Interactions Between Transition Metal Hexafluorides and Xenon," J. D. Webb and E. R. Bernstein.
17. "Absorption and Electronic Raman Scattering Spectra of the $\Gamma_{8g} (^2T_{1g})$ State of IrF_6 at 1.6μ - A Resolution of the Jahn Teller Problem," E. R. Bernstein and J. D. Webb.
18. "The Jahn Teller Effect in the Lowest Charge Transfer State of UF_6 ," E. R. Bernstein, G. R. Meredith and J. D. Webb.
19. "Raman Scattering of Neat and Mixed Crystals of IrF_6 : The Jahn Teller Interaction in the Ground State," E. R. Bernstein and J. D. Webb.
20. "Quadratic Jahn Teller Coupling in Octahedral Systems," E. R. Bernstein and J. D. Webb.
21. "A Ligand Field Theory Analysis of the Spectra of the t_{2g}^3 Levels of IrF_6 ," J. D. Webb and E. R. Bernstein.
22. "Two Photon Spectroscopy of Pyrazine and Triazine," J. D. Webb, K. M. Swift and E. R. Bernstein.

III. ACCOMPLISHMENTS

New results and new work our research has led to includes the following:

- a) Electronic Raman scattering in molecules.
- b) Magnetic phase transition in molecular solids (ReF_6 , IrF_6).
- c) Elucidation of quadratic vibronic coupling (intra- and interstate) - MF_6 , $\text{C}_3\text{N}_3\text{H}_3$.
- d) New insight into photochemical vs. fluorescence yields of excited states ($\text{C}_3\text{N}_3\text{H}_3$, $\text{C}_4\text{N}_2\text{H}_4$, OsO_4).
- e) Spectroscopy of cryogenic liquid solutions and energy transfer.
- f) Phase transition studies in molecular solids.
- g) Polariton behavior in molecular solids.
- h) Elucidation of vibrational mixing (normal mode breakdown) in degenerate electronic states (MF_6 systems).

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